Further work with the Unified Particle-In-Cell and Continuum Method

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Main Ideas

- To understand numerical diffusion due to resetting of particles in the modified numerical algorithm (called Vlasov-PIC or "VP" method), that encompasses the δf particle-in-cell (PIC) method and a continuum method (Vlasov-like), as first explained by Denavit [1].

- The importance:

1. Qualitatively express how *resetting* the particles (*reconstruction*) induces *diffusion.*

2. May help solve the "growing weight problem" in δf particle simulation of plasma turbulence [3, 5].

Vlasov/PIC ("VP") Method

- Algorithm

  – load markers uniformly on phase-space $(x, y, v_\parallel)$ lattice

  – evolve lattice points as if particles

  – *interpolate* δf on the phase-space grid $(x, y, v_\parallel)$

  – **Unique to "VP" method:**

  $*$ redeposit δf marker on original vertex after M time steps

  $\cdot$ call this *reconstruction* or *resetting* of the particles

  $*$ M=1 is Vlasov like, M=(numerical ∞) is δf-PIC and M in between is hybrid

  – obtain density at spatial grid points (x, y) and calculate resulting field

Diffusion Rate Theory

The following is the analytical description of *reconstruction in-duced diffusion*[1]. Consider theory in 1-D.

- After marker particles have been advanced M time-steps they now have positions y_j and the distribution function is

$$f(y) = \sum_j f_j \delta(y - y_j)$$

where j counts all the marker particles.

- Now, reconstruct using weight function:

$$\widetilde{f}(y) = \sum_j f_j \frac{w(y - y_j)}{\Delta y}$$

What is lost with f vs. $\widetilde{f}$

Fourier transform both $\widetilde{f}$ and f and call these the *characteristic* functions of the distribution functions

$$H(k_y) = \int f(y) e^{ik_y y} \, dy$$

$$= \sum_j f_j e^{ik_y y_j}$$

$$\widetilde{H}(l) = \int \widetilde{f}(y) e^{ik_y y} \, dy$$

$$= \int \sum_j f_j \frac{w(y - y_j)}{\Delta y} e^{ik_y y} \, dy \qquad (1)$$

Let $\bar{y} = y - y_j$, then

$$\tilde{H}(k_y) = \int \sum_j f_j \frac{w(\bar{y})}{\Delta y} e^{ik_y(\bar{y}+y_j)} d\bar{y}$$

$$= \sum_j f_j e^{ik_y y_j} \cdot \underbrace{\int \frac{w(\bar{y})}{\Delta y} e^{ik_y \bar{y}} d\bar{y}}_{W(k_y)}$$

So,

$$\tilde{H}(k_y) = W(k_y) \sum_j f_j e^{ik_y y_j} \tag{2}$$

Thus comparing (1) and (2) we get:

$$\tilde{H}(k_y) = W(k_y) H(k_y) \tag{3}$$

What is lost with $\tilde{f}$ vs. f (cont.)

So we have the characteristic function:

$$\tilde{H}(k_y) = W(k_y) H(k_y)$$

and if we define:

$$D(k_y) = 1 - W(k_y)$$

then,

$$\tilde{H}(k_y) = (1 - D(k_y)) H(k_y).$$

If we reconstruct m-times then, *by induction,*

$$\tilde{H}(k_y; m) = H(k_y; m = 0) \cdot (1 - D(k_y))^m.$$

What is lost with $\tilde{f}$ vs. f (cont.)

Consider $\dfrac{k_y \cdot \Delta y}{\pi} \ll 1$, then,

$$(1 - D(k_y))^m \cong e^{-m \cdot D(k_y)},$$

thus,

$$\tilde{H}(k_y; m) \cong H(k_y; m = 0) \cdot e^{-m \cdot D(k_y)}. \qquad (4)$$

So, in Fourier space, we see the effect of the reconstruction as a diffusion process.
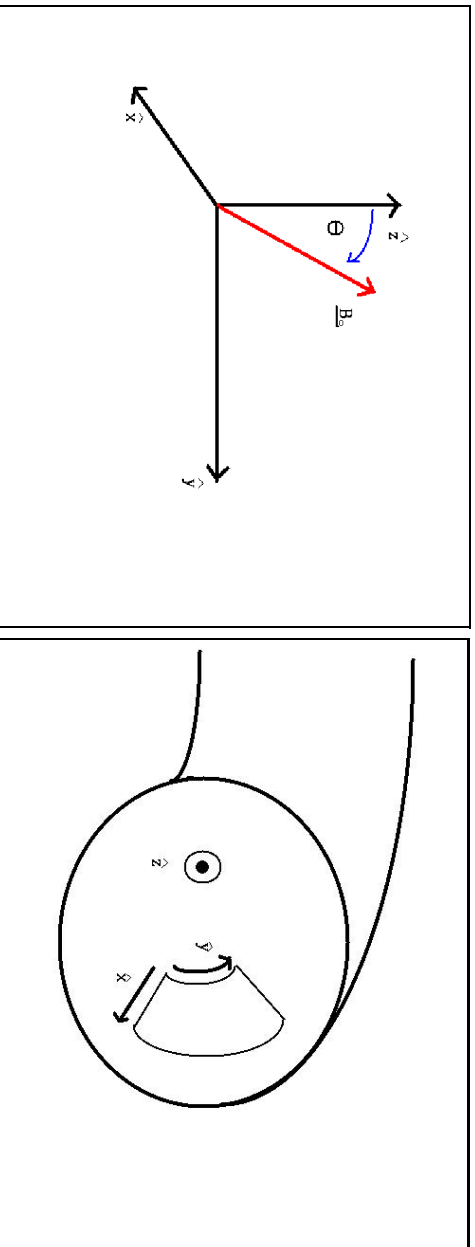
Problem we are studying.

Figure 1: "Slab" geometry with temperature and density gradient in $-\hat{\mathbf{x}}$

- Strong Magnetic Field

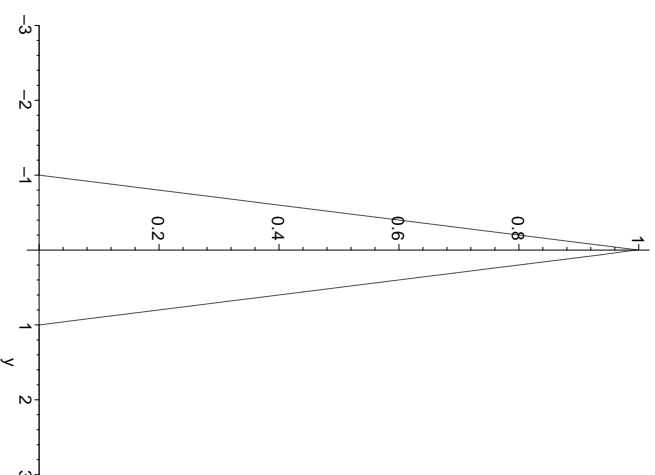$$\hat{\mathbf{B}} = B_0\hat{\mathbf{z}} + \theta\hat{\mathbf{y}}, \theta << 1$$

- Evolution Equation

$$[\partial_t + \mathbf{v}_\parallel \cdot \nabla_\parallel]\delta f = 0$$

Calculation of $D_1(k_y) = 1 - W_1(k_y)$

Linear weight function:

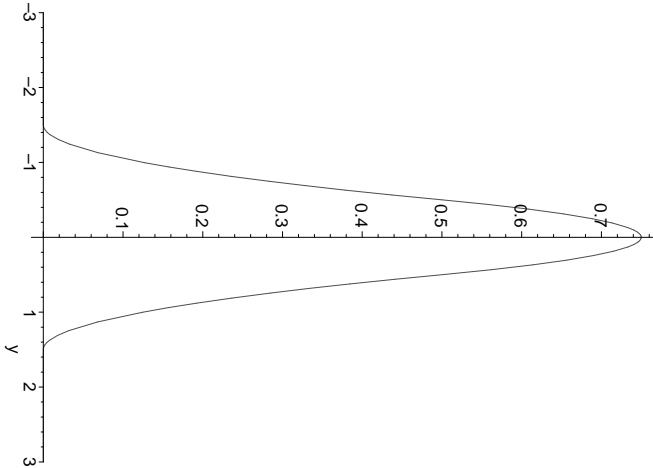$$w_1(y) = \begin{cases} 1 - |y| & |y| \leq 1 \\ 0 & \text{elsewhere} \end{cases}$$

The Fourier Transform of such a piecewise-continuous function is

$$W_1(k_y) = -2\frac{\cos(k_y) - 1}{k_y^2}$$

Calculation of $D_2(k_y) = 1 - W_1(k_y)$

Quadratic weight function [4]

$$w_2(y) = \begin{cases} \frac{3}{4} - y^2 & |y| \le \frac{1}{2} \\ \frac{1}{2}\left(\frac{3}{2} - |y|\right)^2 & \frac{1}{2} \le |y| \text{ and } |y| \le \frac{3}{2} \\ 0 & \text{elsewhere} \end{cases}$$

The Fourier Transform of such a piecewise-smooth function is

$$W_2(k_y) = -2\frac{\sin(\frac{3}{2}k_y) - 3\sin(\frac{1}{2}k_y)}{k_y^3},$$

Simulation Echoes

We will use simulation echoes as an indicator of reconstruction induced diffusion.

The qualities of the echoes are:

- existence because system has no external fields

- which allows for the distribution to reorder

- echo period $\tau = \frac{l_y}{\theta \cdot \Delta v}$

For our simulation, length of $y = 16$, $\Delta v = \frac{1}{8}$, and $\theta = .0128$, resulting in $\tau = 10000$.

We analyzed the $(1,1)$ mode, which is equivalent to

$$k_y = \frac{2\pi}{l_y} \cdot \Delta y = \frac{\pi}{16}.$$
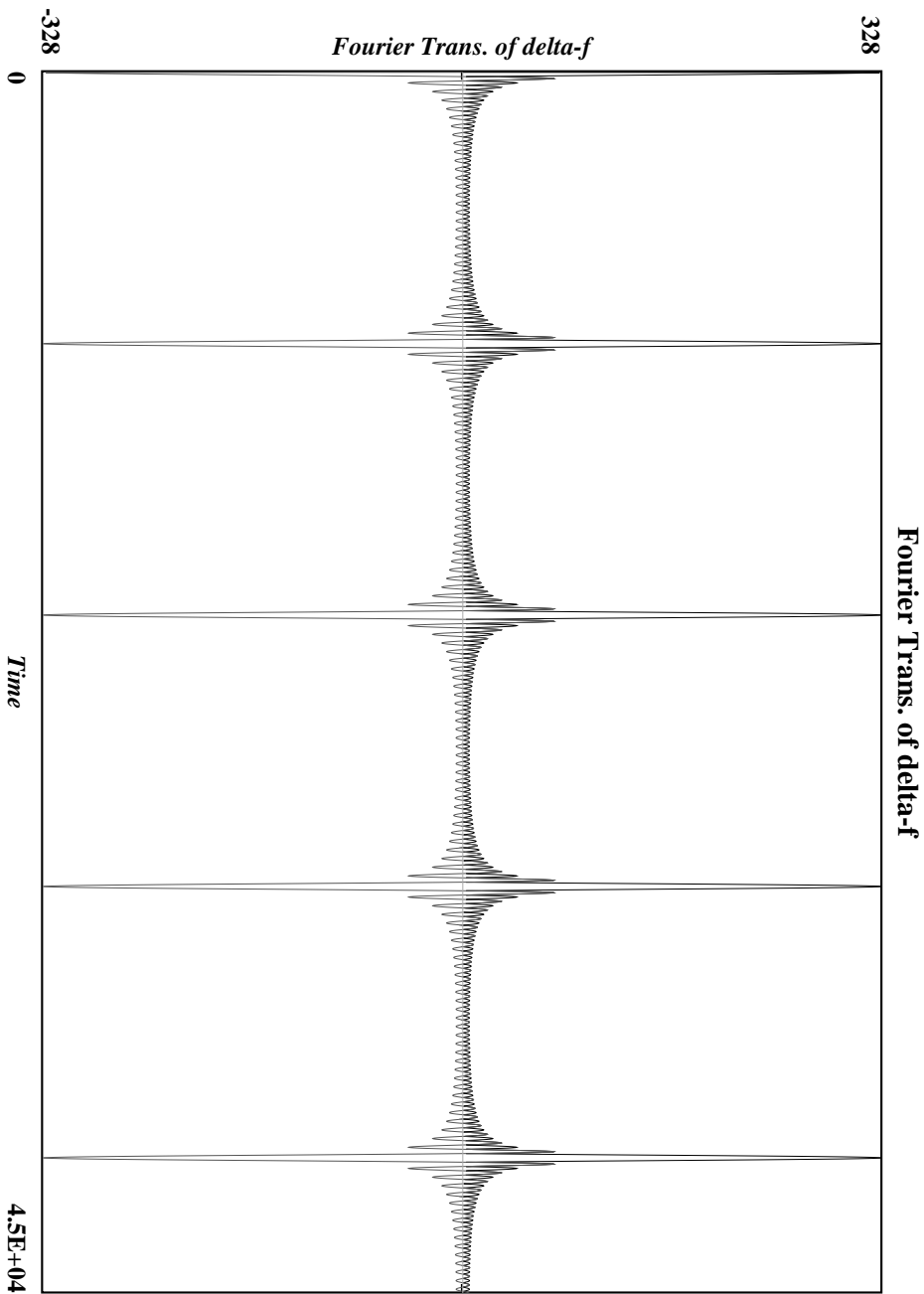
Example of simulation echoes, using w_2.

Not resetting the particles results in no diffusion.

Fourier Trans. of delta-f

Figure 2: M=∞, we never reset the particles (PIC method).

Note that there is little diffusion.

Reconstruction diffusion, $M=600$, using w_2.
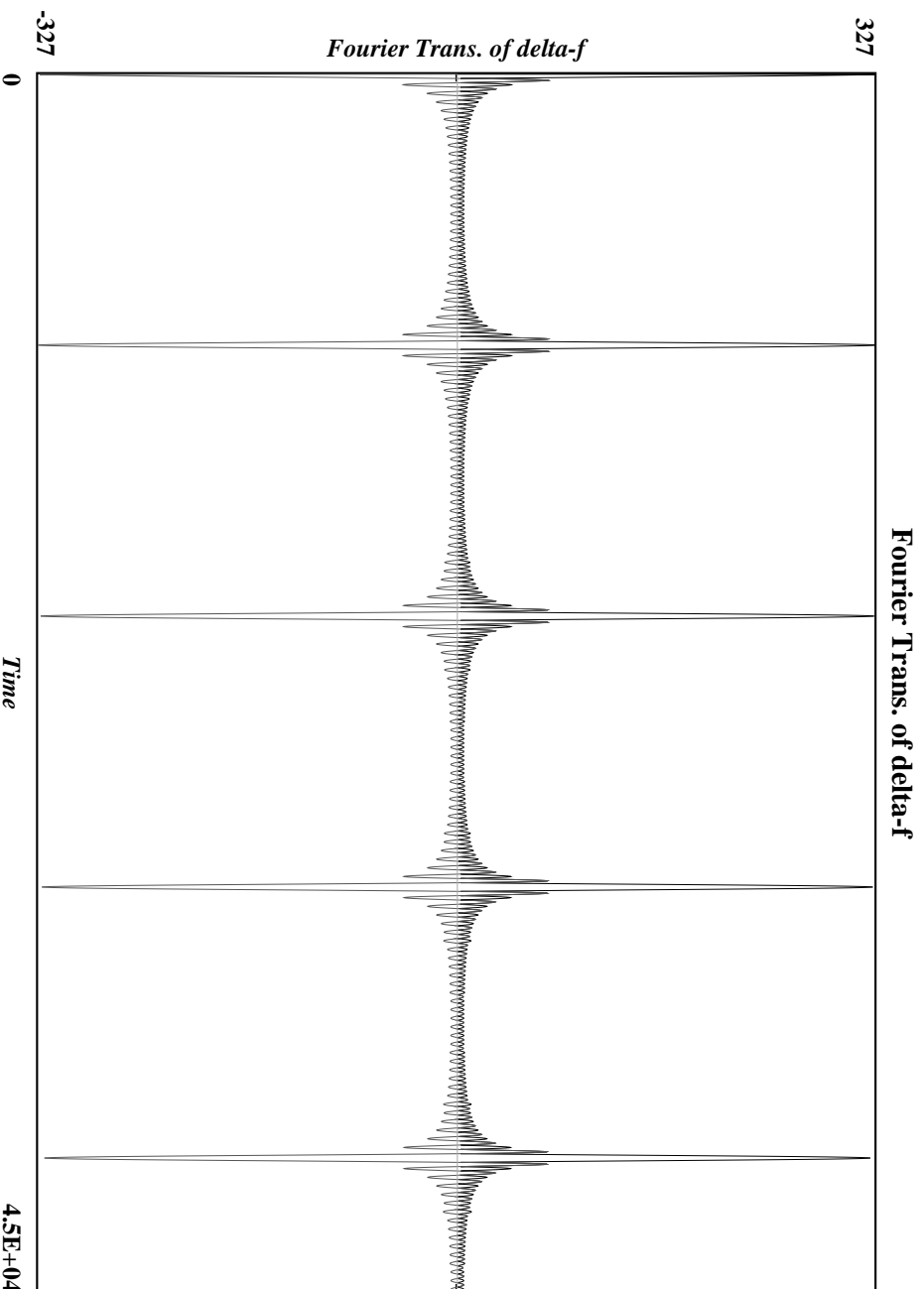
Figure 3: We reset the particles every 6000[time], 1 between each echo.

Reconstruction diffusion, M=100, using w_2.

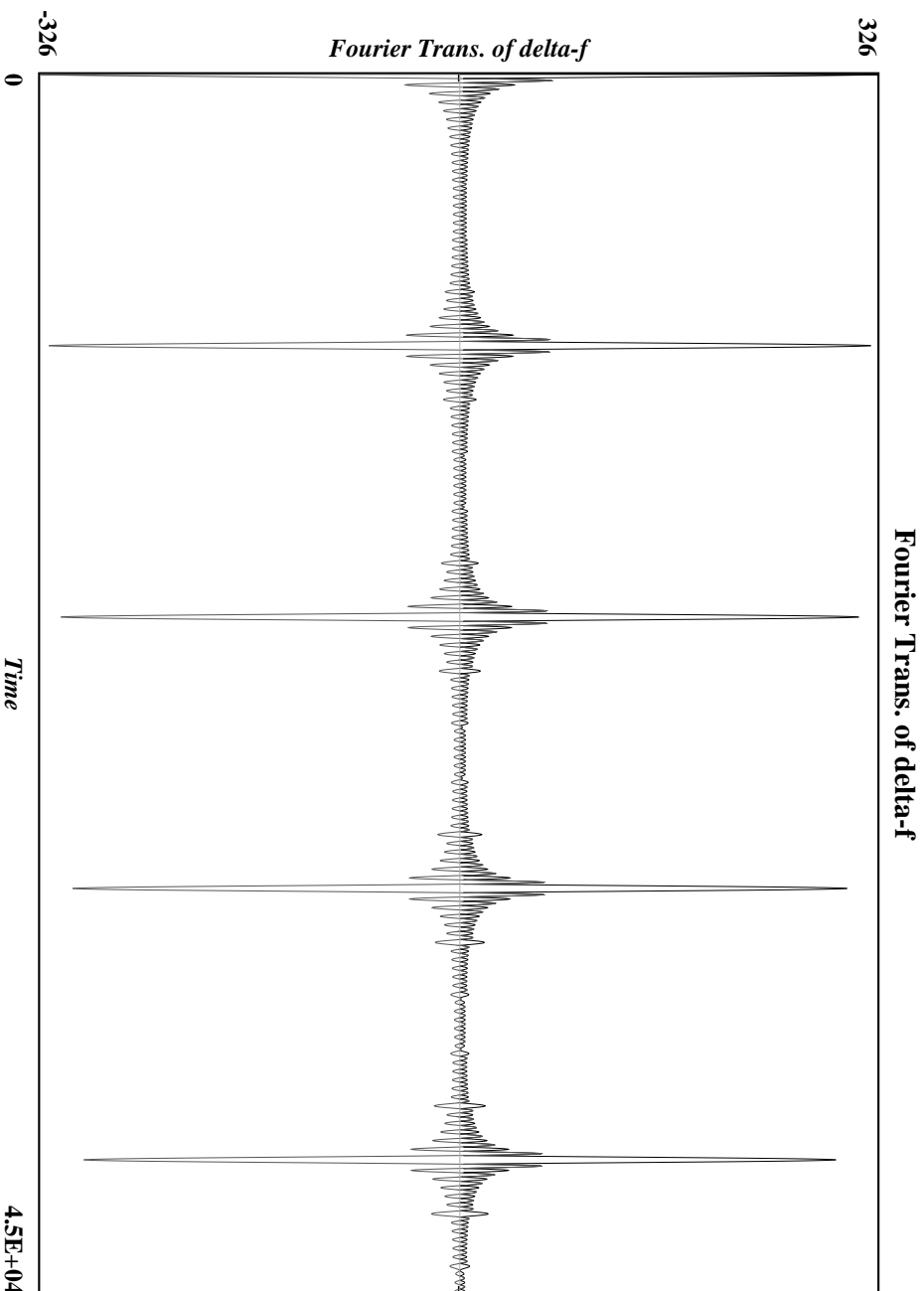**Fourier Trans. of delta-f**

Figure 4: We reset the particles every 1000[time], 10 times between each echo.

We see the result of such resets as a decrees of the echo amplitude.

Reconstruction diffusion diffusion, M=20 , using w2.

Fourier Trans. of delta-f

Fourier Trans. of delta-f
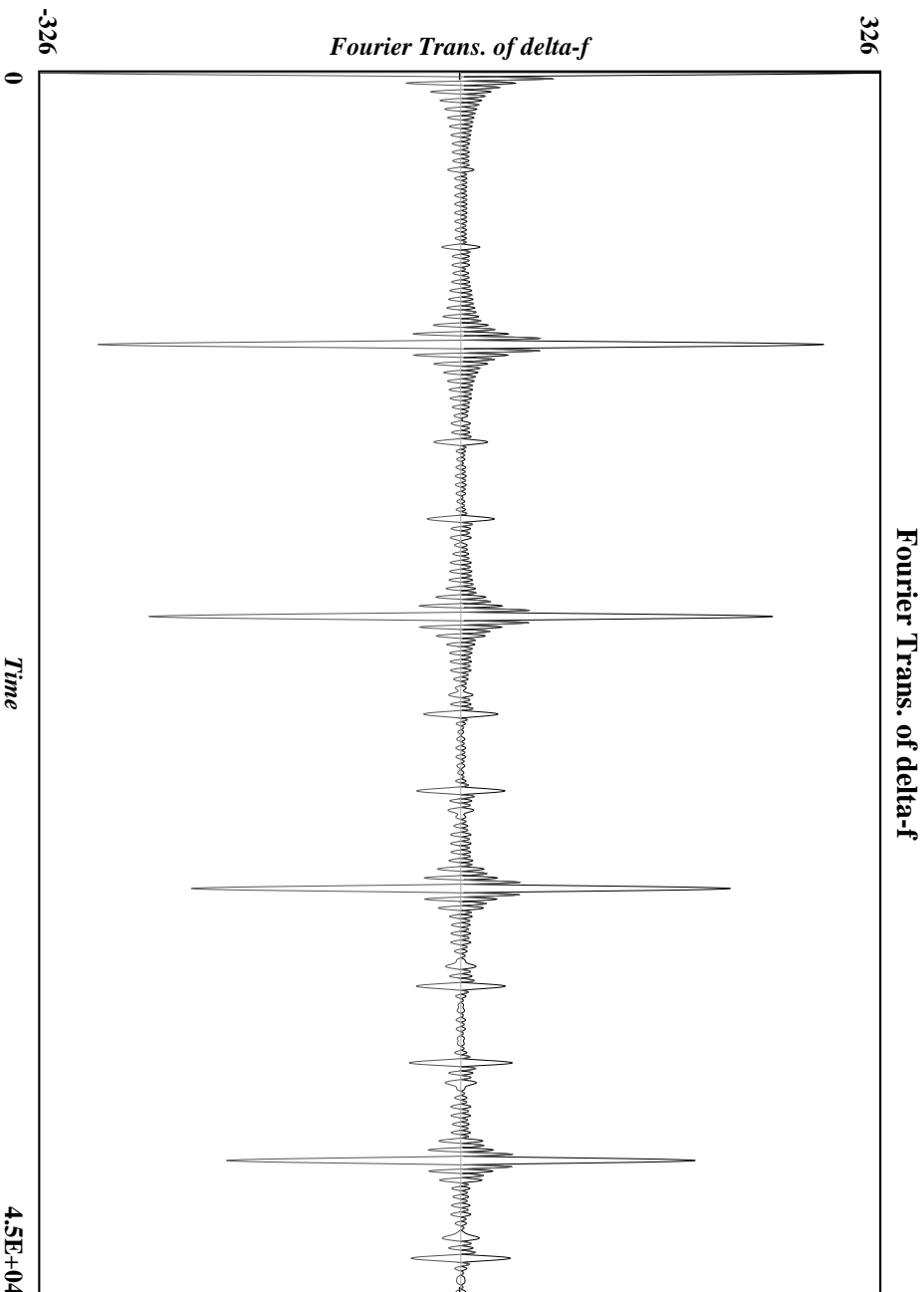
326

-326

0

Time

4.5E+04

Figure 5: We reset the particles every 200[time],50 times between each echo.

We now see more diffusion due to the often resetting of particles.

Reconstruction diffusion, M=1, using w_2.

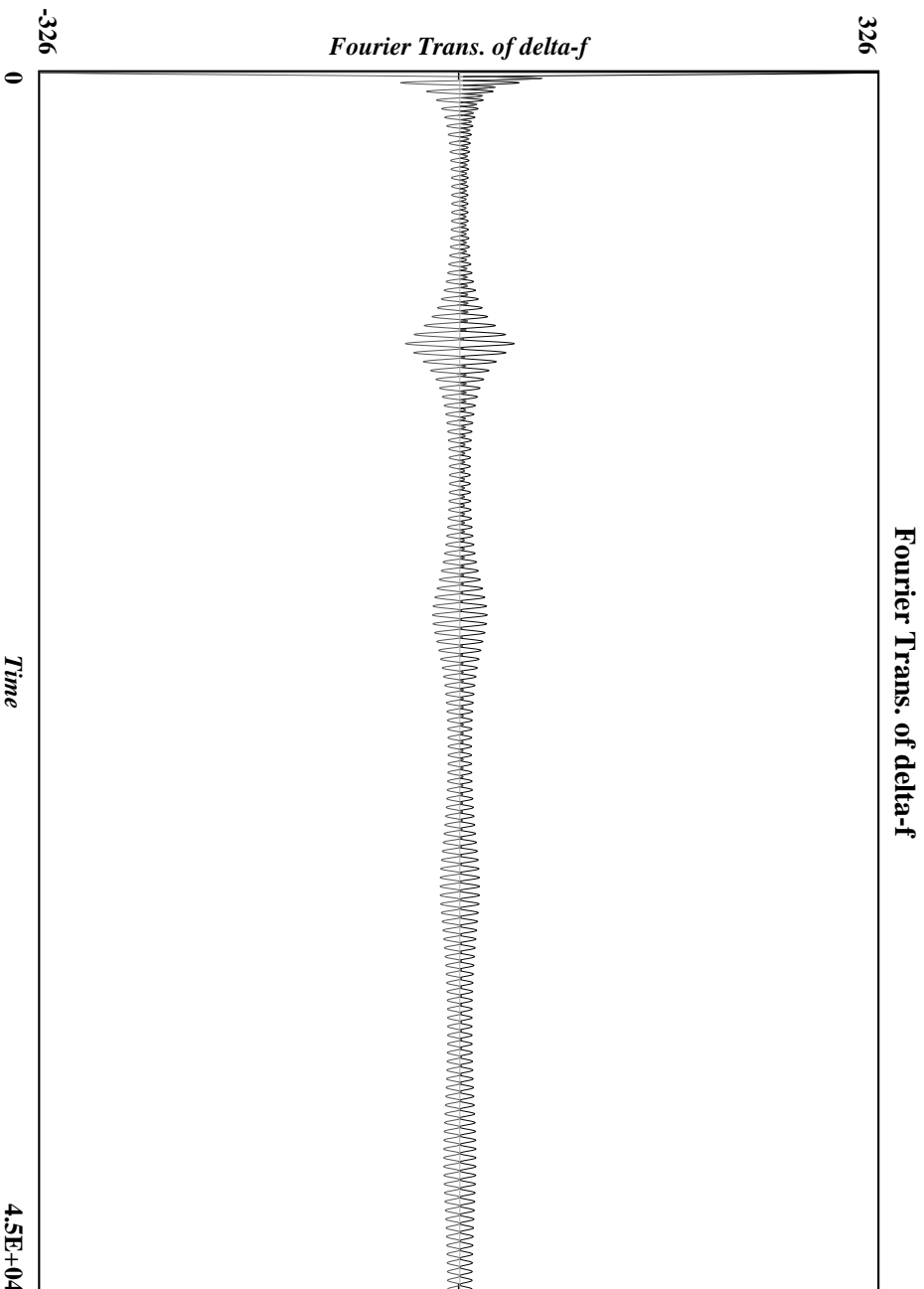**Fourier Trans. of delta-f**

Figure 6: We reset the particles every 10[time], 1000 times between each echo.

We see a great decrease in the echo amplitude due to many resets.

Induced Diffusion: $e^{-D(k_y)*\frac{t_{echo}}{\Delta t.M}}$

Theory	$D_1(k_y) = 3.2086361 \times 10^{-3}$	$D_2(k_y) = 4.8090913 \times 10^{-3}$
m: times reset	$D_1(k_y) \times 10^{-3}$	$D_2(k_y) \times 10^{-3}$
1000	2.0456910×10^{-3}	2.04461812×10^{-3}
200	2.9414892×10^{-3}	2.9280185×10^{-3}
100	3.0385852×10^{-3}	3.0094981×10^{-3}
50	3.1303167×10^{-3}	3.0689835×10^{-3}
20	3.0524134×10^{-3}	2.9017329×10^{-3}
10	2.7191638×10^{-3}	3.0187368×10^{-3}
m=1,M=600	3.6356449×10^{-3}	1.8238425×10^{-3}
m=0,M=1000	4.3511390×10^{-6}	5.3644180×10^{-7}

Table 1: Simulation values from ratio of echo amplitudes
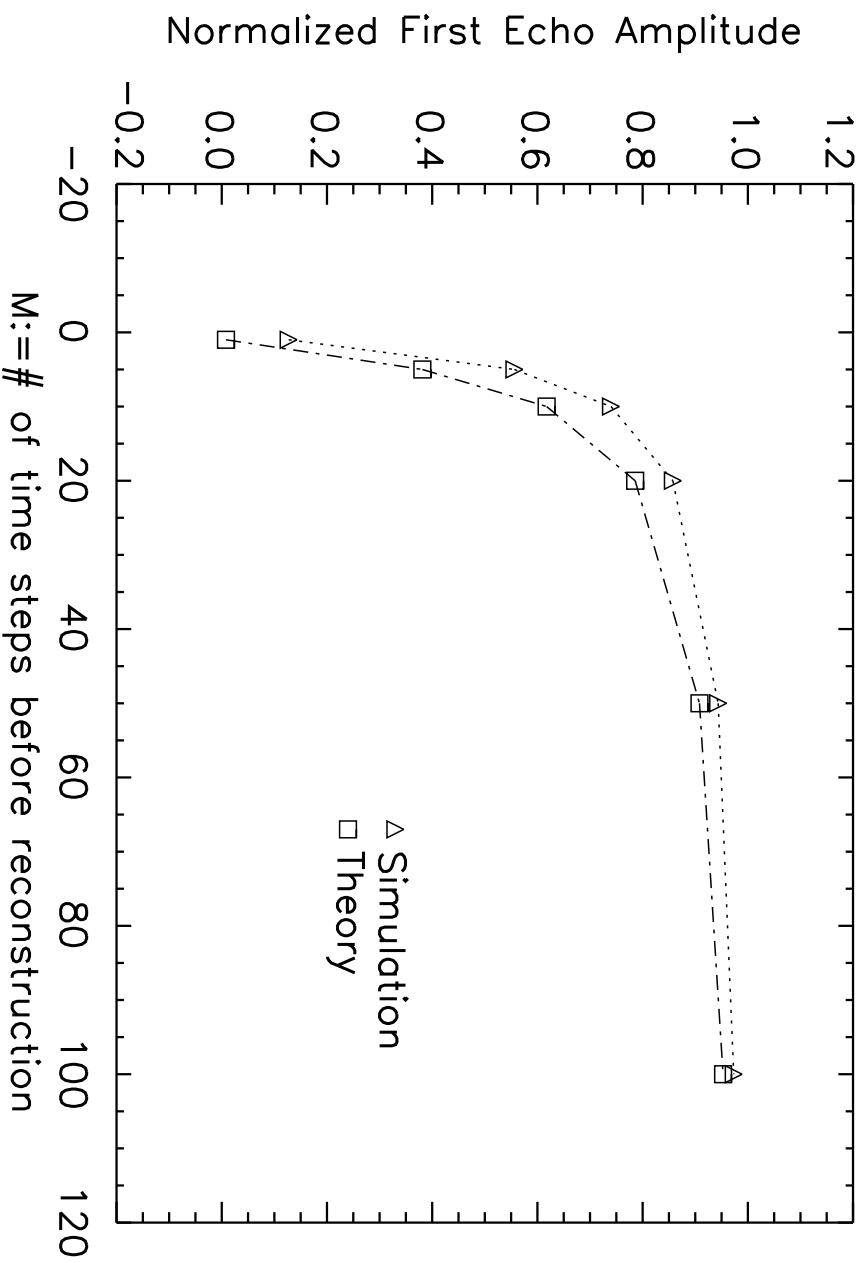
Results of diffusion due to reconstruction

Figure 7: Reconstructing less induces much less diffusion. This is for the quadratic interpolation.

The less times we reconstruct gives less diffusion.

Conclusion

- We have a qualitative way to describe *repeated resetting of the particles* induced numerical diffusion.

- What is next?

  – Denavit's analysis predicts more diffusion from the higher order interpolation reconstruction schemes. Understand discrepancy with simulation data.

  – Further investigate the nature of the plasma simulation echoes and influence by such reconstruction.

References

[1] Denavit, J. Comp. Phys. **9** 75 (1972)

[2] Cheng and Knorr, JCP **22** 330 (1976)

[3] Hu and Krommes, Phys. Plasmas **1** 3211 (1994)

[4] Hockney and Eastwood, *Computer Simulation Using Particles*, 137 (1999)

[5] Brunner, Valeo and Krommes, Phys. Plasmas **6** 4504 (1999)

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[7] S.E. Parker, W. Dorland, R. Santoro, M. Beer, Q. Liu, W. Lee and G. Hammet, Phys. Plasmas **1** (5) 1461 (1994)